

chain nodes :

7 10 16 18

ring nodes :

1 2 3 4 5 6 11 12 13 14 15

chain bonds :

2-7 7-10

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

7-10

exact bonds :

2-7 11-12 11-15 12-13 13-14 14-15

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

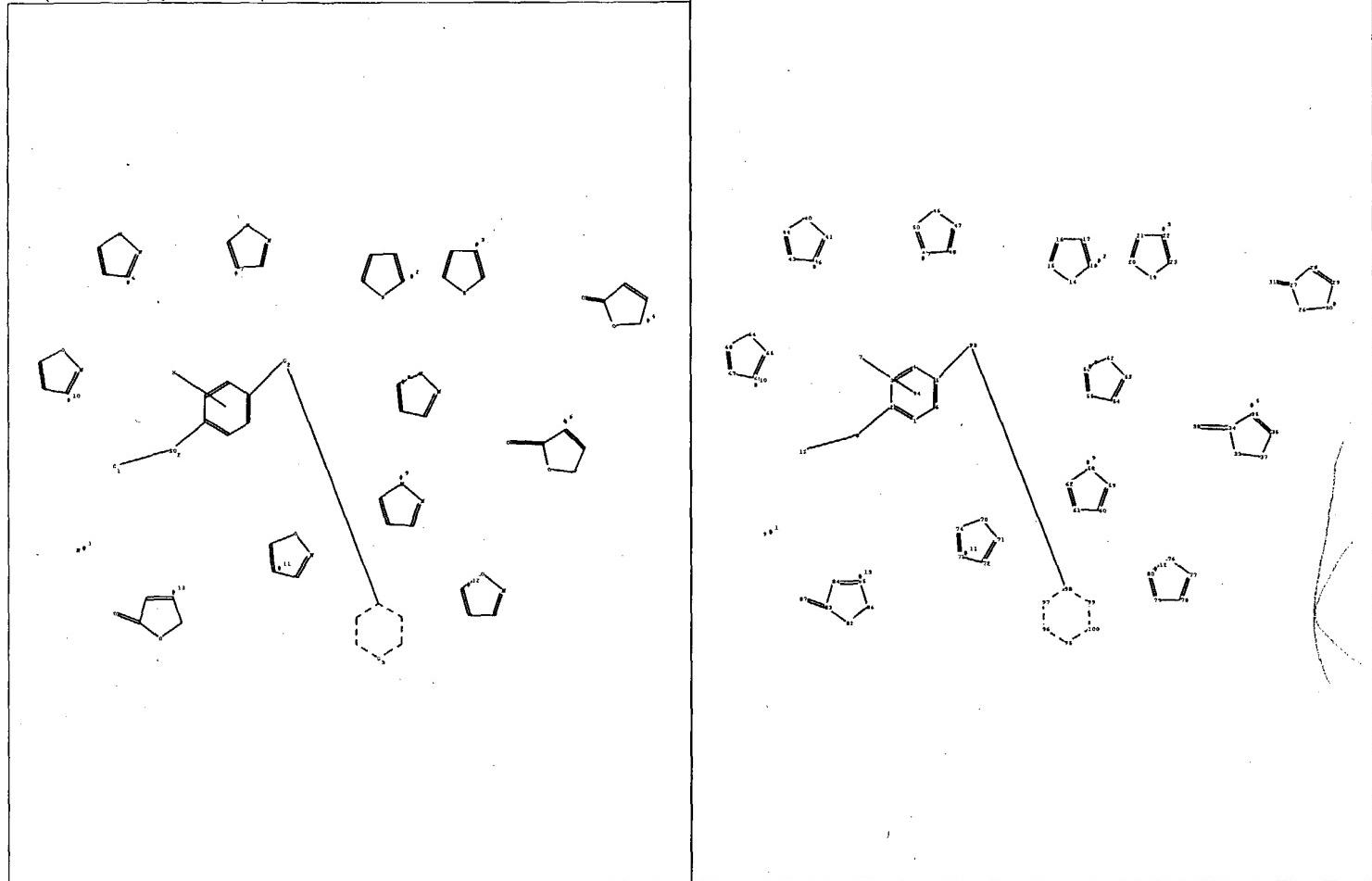
isolated ring systems :

containing 1 : 11 :

G1:Ak,NH2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 10:CLASS 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:Atom 19:CLASS



chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1	2	3	4	5	6	14	15	16	17	18	19	20	21	22	23	26	27	28	29	30	33	34	35
36	37	40	41	42	43	44	46	47	48	49	49	50	52	53	54	55	56	58	59	60	61	62	
64	65	66	67	68	70	71	72	73	74	76	77	78	79	80	82	83	84	85	86	95	96		
97	98	99	100																				

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-98

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21										
21-22	22-23	26-27	26-30	27-28	28-29	29-30	33-34	33-37	34-35	35-36	36-37	40-41											
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-56	53-54	54-55											
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-74											
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	84-85	85-86											
95-96	95-100	96-97	97-98	98-99	99-100																		

exact/norm bonds :

5-93	8-12	27-31	34-38	40-41	40-44	41-42	46-47	46-50	47-48	52-53	52-56	53-54											
58-59	58-62	59-60	65-66	71-72	77-78	83-87	93-98	95-96	95-100	96-97	97-98												
98-99	99-100																						

exact bonds :

2-8	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21	21-22	22-23	26-27	26-30											
27-28	28-29	29-30	33-34	33-37	34-35	35-36	36-37	42-43	43-44	48-49	49-50	54-55											
55-56	60-61	61-62	64-65	64-68	66-67	67-68	70-71	70-74	72-73	73-74	76-77	76-80											
78-79	79-80	82-83	82-86	83-84	84-85	85-86																	

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

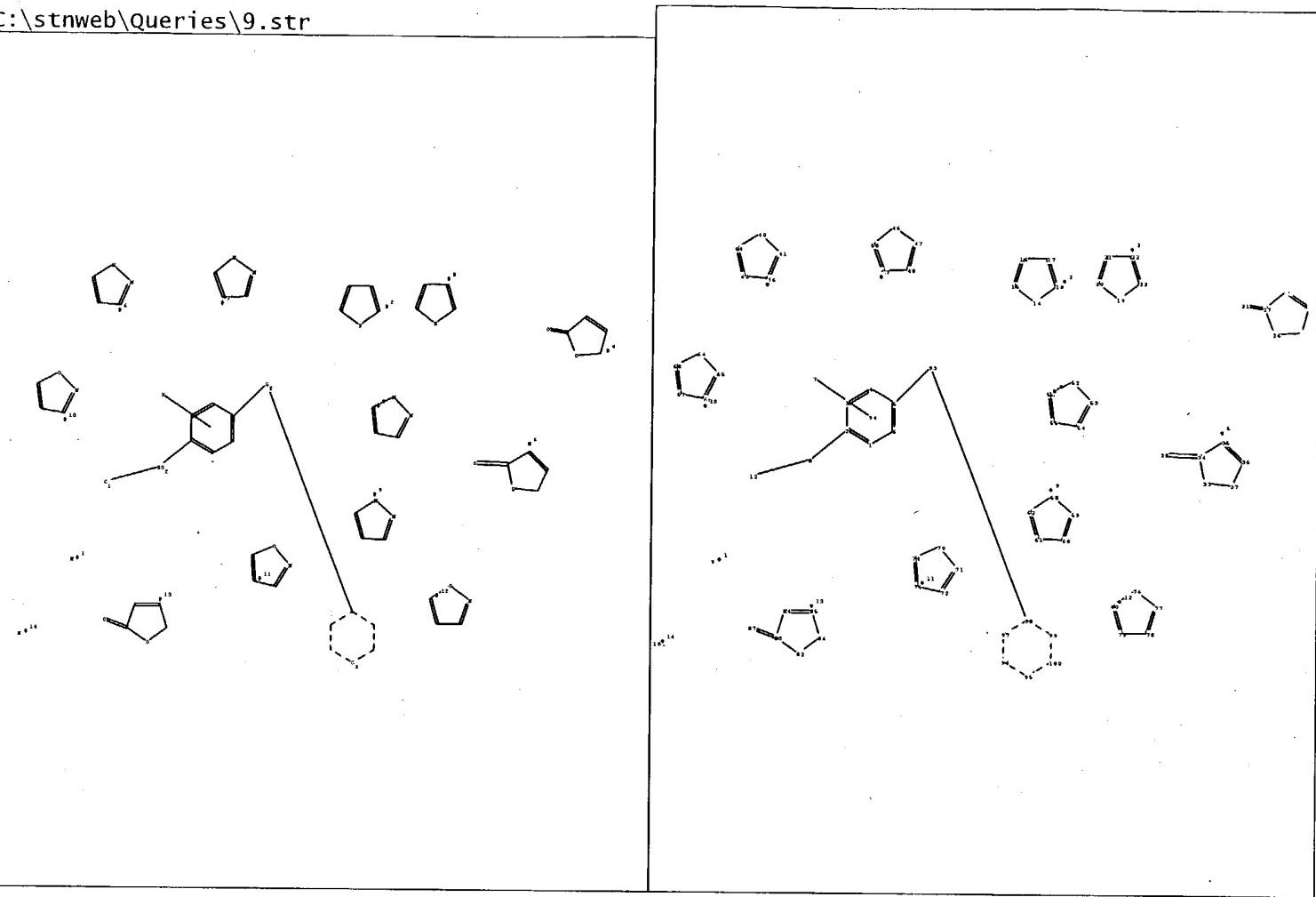
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 100:Atom



chain nodes :

7 8 9 12 31 38 87 93 101

ring nodes :

1	2	3	4	5	6	14	15	16	17	18	19	20	21	22	23	26	27	28	29	30	33	34	35
36	37	40	41	42	43	44	46	47	48	49	49	50	52	53	54	55	56	58	59	60	61	62	
64	65	66	67	68	70	71	72	73	74	76	77	78	79	80	82	83	84	85	86	95	96		
97	98	99	100																				

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-98

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	14-15	14-18	14-19	15-16	16-17	16-18	17-18	19-20	19-23	20-21				
21-22	22-23	26-27	26-30	27-28	28-29	29-30	33-34	33-37	34-35	35-36	36-37	40-41							
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-56	53-54	54-55							
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-74							
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	84-85	85-86							
95-96	95-100	96-97	97-98	98-99	99-100														

exact/norm bonds :

5-93	8-12	27-31	34-38	40-41	40-44	41-42	46-47	46-50	47-48	52-53	52-56	53-54
58-59	58-62	59-60	65-66	71-72	77-78	83-87	93-98	95-96	95-100	96-97	97-98	
98-99	99-100											

exact bonds :

2-8	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21	21-22	22-23	26-27	26-30
27-28	28-29	29-30	33-34	33-37	34-35	35-36	36-37	42-43	43-44	48-49	49-50	54-55
55-56	60-61	61-62	64-65	64-68	66-67	67-68	70-71	70-74	72-73	73-74	76-77	76-80
78-79	79-80	82-83	82-86	83-84	84-85	85-86						

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

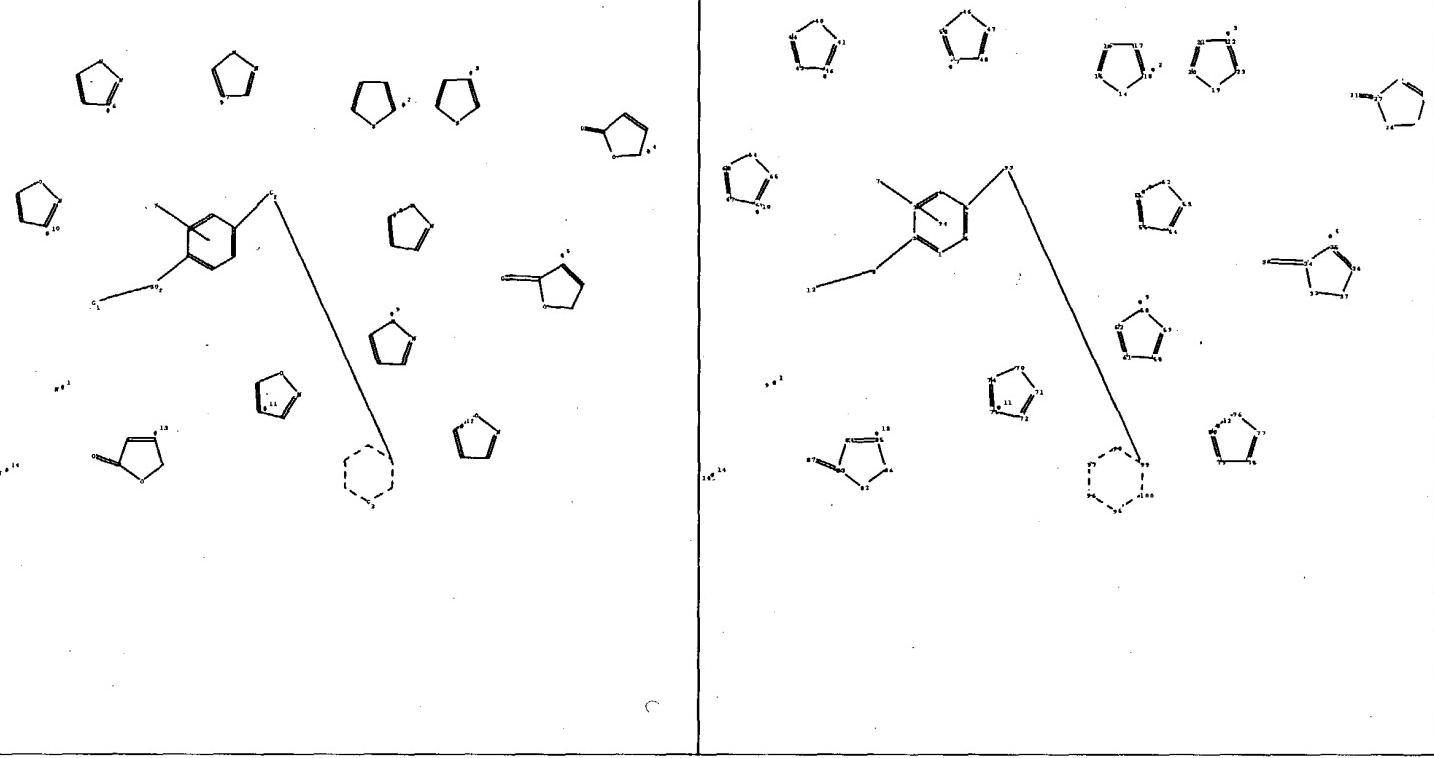
:CH3,Et,[*1]

:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,[*14]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 100:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93 101

ring nodes :

1	2	3	4	5	6	14	15	16	17	18	19	20	21	22	23	26	27	28	29	30	33	34	35
36	37	40	41	42	43	44	46	47	48	49	49	50	52	53	54	55	56	58	59	60	61	62	
64	65	66	67	68	70	71	72	73	74	76	77	78	79	80	82	83	84	85	86	95	96		
97	98	99	100																				

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-99

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21									
21-22	22-23	26-27	26-30	27-28	28-29	29-30	33-34	33-37	34-35	35-36	36-37	40-41										
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-56	53-54	54-55										
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-74										
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	84-85	85-86										
95-96	95-100	96-97	97-98	98-99	99-100																	

exact/norm bonds :

5-93	8-12	27-31	34-38	40-41	40-44	41-42	46-47	46-50	47-48	52-53	52-56	53-54										
58-59	58-62	59-60	65-66	71-72	77-78	83-87	93-99	95-96	95-100	96-97	97-98											
98-99	99-100																					

exact bonds :

2-8	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21	21-22	22-23	26-27	26-30										
27-28	28-29	29-30	33-34	33-37	34-35	35-36	36-37	42-43	43-44	48-49	49-50	54-55										
55-56	60-61	61-62	64-65	64-68	66-67	67-68	70-71	70-74	72-73	73-74	76-77	76-80										
78-79	79-80	82-83	82-86	83-84	84-85	85-86																

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

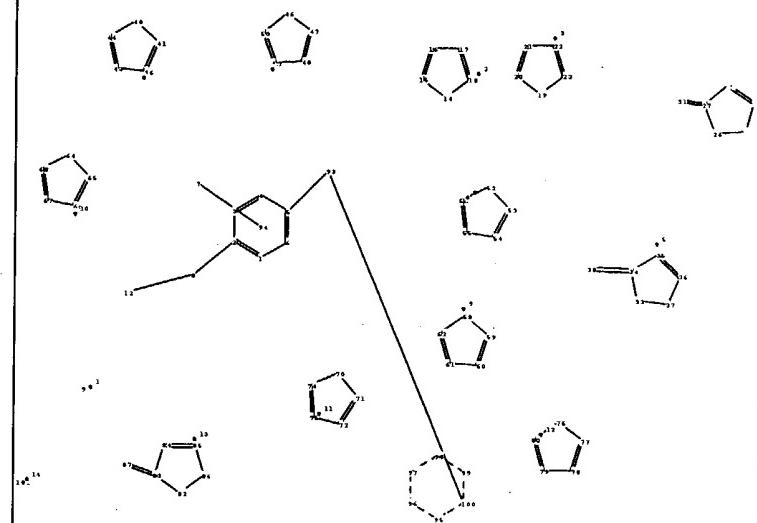
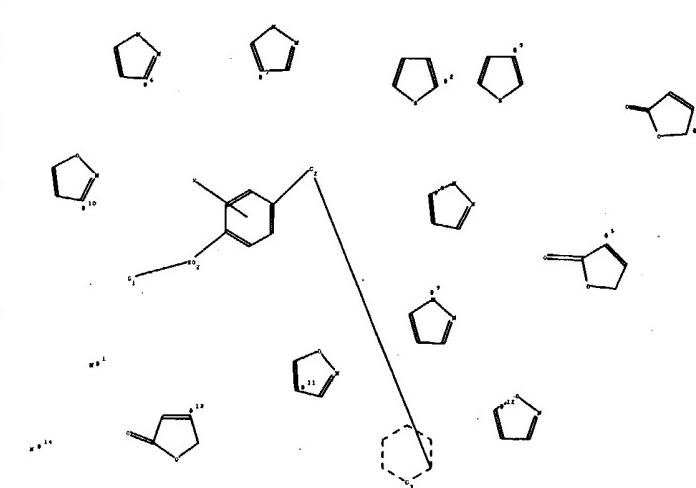
1:CH3,Et,[*1]

2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:c,[*14]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
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37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
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85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 100:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93 101

ring nodes :

1	2	3	4	5	6	14	15	16	17	18	19	20	21	22	23	26	27	28	29	30	33	34	35
36	37	40	41	42	43	44	46	47	48	49	50	52	53	54	55	56	58	59	60	61	62		
64	65	66	67	68	70	71	72	73	74	76	77	78	79	80	82	83	84	85	86	95	96		
97	98	99	100																				

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-100

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21									
21-22	22-23	26-27	26-30	27-28	28-29	29-30	33-34	33-37	34-35	35-36	36-37	40-41										
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-56	53-54	54-55										
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-74										
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	84-85	85-86										
95-96	95-100	96-97	97-98	98-99	99-100																	

exact/norm bonds :

5-93	8-12	27-31	34-38	40-41	40-44	41-42	46-47	46-50	47-48	52-53	52-56	53-54										
58-59	58-62	59-60	65-66	71-72	77-78	83-87	93-100	95-96	95-100	96-97	97-98											
98-99	99-100																					

exact bonds :

2-8	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21	21-22	22-23	26-27	26-30										
27-28	28-29	29-30	33-34	33-37	34-35	35-36	36-37	42-43	43-44	48-49	49-50	54-55										
55-56	60-61	61-62	64-65	64-68	66-67	67-68	70-71	70-74	72-73	73-74	76-77	76-80										
78-79	79-80	82-83	82-86	83-84	84-85	85-86																

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

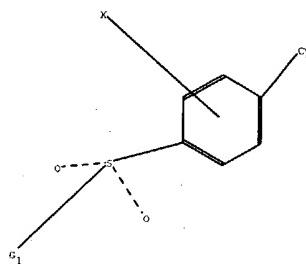
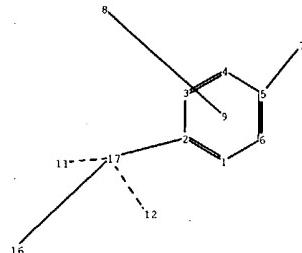
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

c,[*14]

ch level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 100:Atom 101:CLASS

 $\text{N}^{\theta 1}$  $\text{L}^{\theta 1}$

chain nodes :

7 8 11 12 13 16 17

ring nodes :

1 2 3 4 5 6

chain bonds :

2-17 5-7 11-17 12-17 16-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

2-17 5-7 11-17 12-17 16-17

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

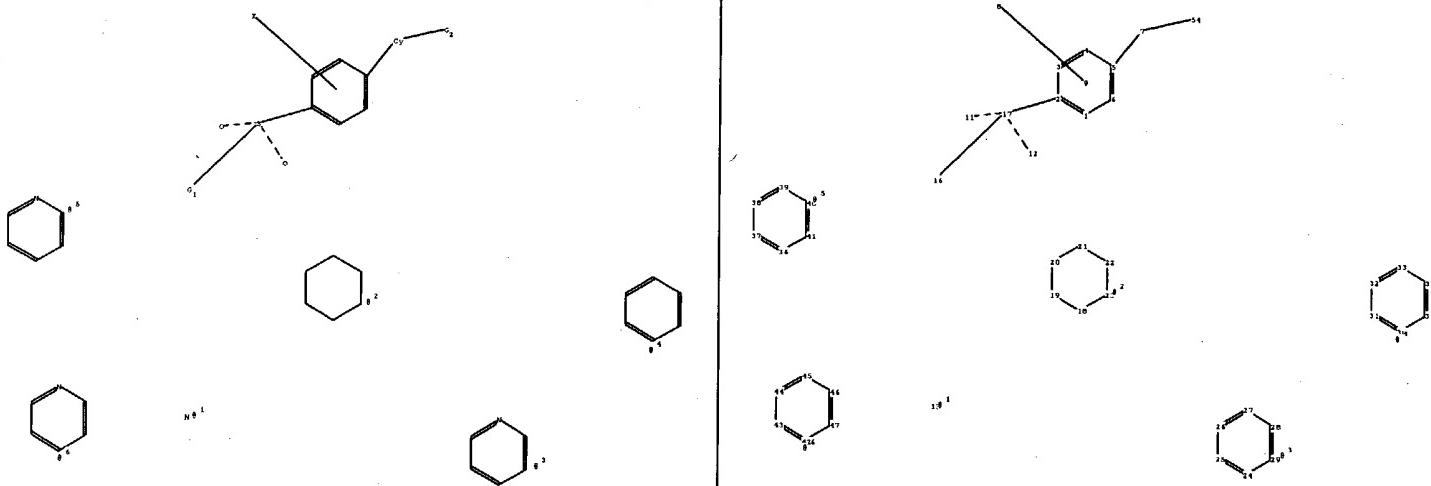
isolated ring systems :

containing 1 :

G1:CH3,Et,[*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS 16:CLASS 17:CLASS



chain nodes :

7 8 11 12 13 16 17 54

ring nodes :

1 2 3 4 5 6 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35
36 37 38 39 40 41 42 43 44 45 46 47

chain bonds :

2-17 5-7 7-54 11-17 12-17 16-17

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23 24-25 24-29
25-26 26-27 27-28 28-29 30-31 30-35 31-32 32-33 33-34 34-35 36-37 36-41 37-38
38-39 39-40 40-41 42-43 42-47 43-44 44-45 45-46 46-47

exact/norm bonds :

2-17 5-7 7-54 11-17 12-17 16-17

exact bonds :

18-19 18-23 19-20 20-21 21-22 22-23

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 24-25 24-29 25-26 26-27 27-28 28-29 30-31 30-35
31-32 32-33 33-34 34-35 36-37 36-41 37-38 38-39 39-40 40-41 42-43 42-47 43-44
44-45 45-46 46-47

isolated ring systems :

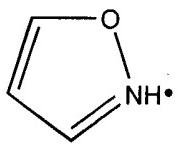
containing 1 : 18 : 24 : 30 : 36 : 42 :

G1:CH3,Et,[*1]

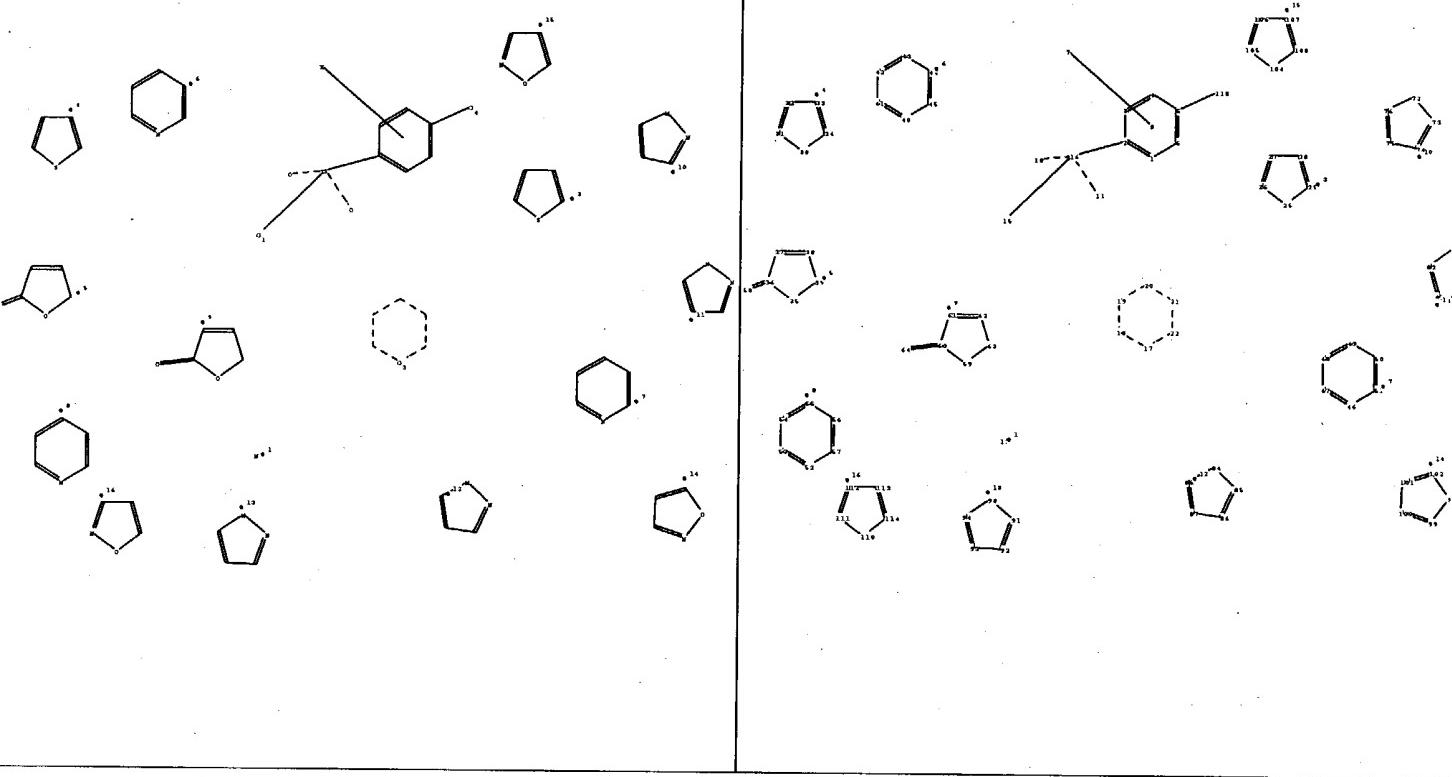
G2:[*2],[*3],[*4],[*5],[*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:CLASS 9:CLASS 11:CLASS
12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom
43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 54:CLASS



isoxazolyl



chain nodes :

7 10 11 12 15 16 58 64 118

ring nodes :

1	2	3	4	5	6	17	18	19	20	21	22	25	26	27	28	29	30	31	32	33	34	35	36
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	59		
60	61	62	63	72	73	74	75	76	78	79	80	81	82	84	85	86	87	88	90	91	92		
93	94	98	99	100	101	102	104	105	106	107	108	110	111	112	113	114							

chain bonds :

2-16 5-118 10-16 11-16 15-16 36-58 60-64

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	17-18	17-22	18-19	19-20	20-21	21-22	25-26	25-29											
26-27	27-28	28-29	30-31	30-34	31-32	32-33	33-34	35-36	35-39	36-37	37-38	38-39												
40-41	40-45	41-42	42-43	43-44	44-45	46-47	46-51	47-48	48-49	49-50	50-51	52-53												
52-57	53-54	54-55	55-56	56-57	59-60	59-63	60-61	61-62	62-63	72-73	72-76	73-74												
74-75	75-76	78-79	78-82	79-80	80-81	81-82	84-85	84-88	85-86	86-87	87-88	90-91	90-94	91-92	92-93	93-94	98-99	98-102	99-100	100-101	101-102	104-105	104-108	
90-94	91-92	92-93	93-94	98-99	98-102	99-100	100-101	101-102	104-105	104-108	105-106	106-107	107-108	110-111	111-112	112-113	113-114							

exact/norm bonds :

2-16	5-118	10-16	11-16	15-16	17-18	17-22	18-19	19-20	20-21	21-22	25-26	25-29												
26-27	27-28	28-29	30-31	30-34	31-32	32-33	33-34	35-36	35-39	36-37	36-58	37-38												
38-39	59-60	59-63	60-61	60-64	61-62	62-63	72-73	72-76	73-74	74-75	75-76	78-79												
78-82	79-80	80-81	81-82	84-85	84-88	85-86	86-87	87-88	90-91	90-94	91-92	92-93												
93-94	98-99	98-102	99-100	100-101	101-102	104-105	104-108	105-106	106-107															
107-108	110-111	110-114	111-112	112-113	113-114																			

normalized bonds :

1-2	1-6	2-3	3-4	4-5	5-6	40-41	40-45	41-42	42-43	43-44	44-45	46-47	46-51											
47-48	48-49	49-50	50-51	52-53	52-57	53-54	54-55	55-56	56-57															

isolated ring systems :

containing 1 : 17 : 25 : 30 : 35 : 40 : 46 : 52 : 59 : 72 : 78 : 84 : 90 : 110 :

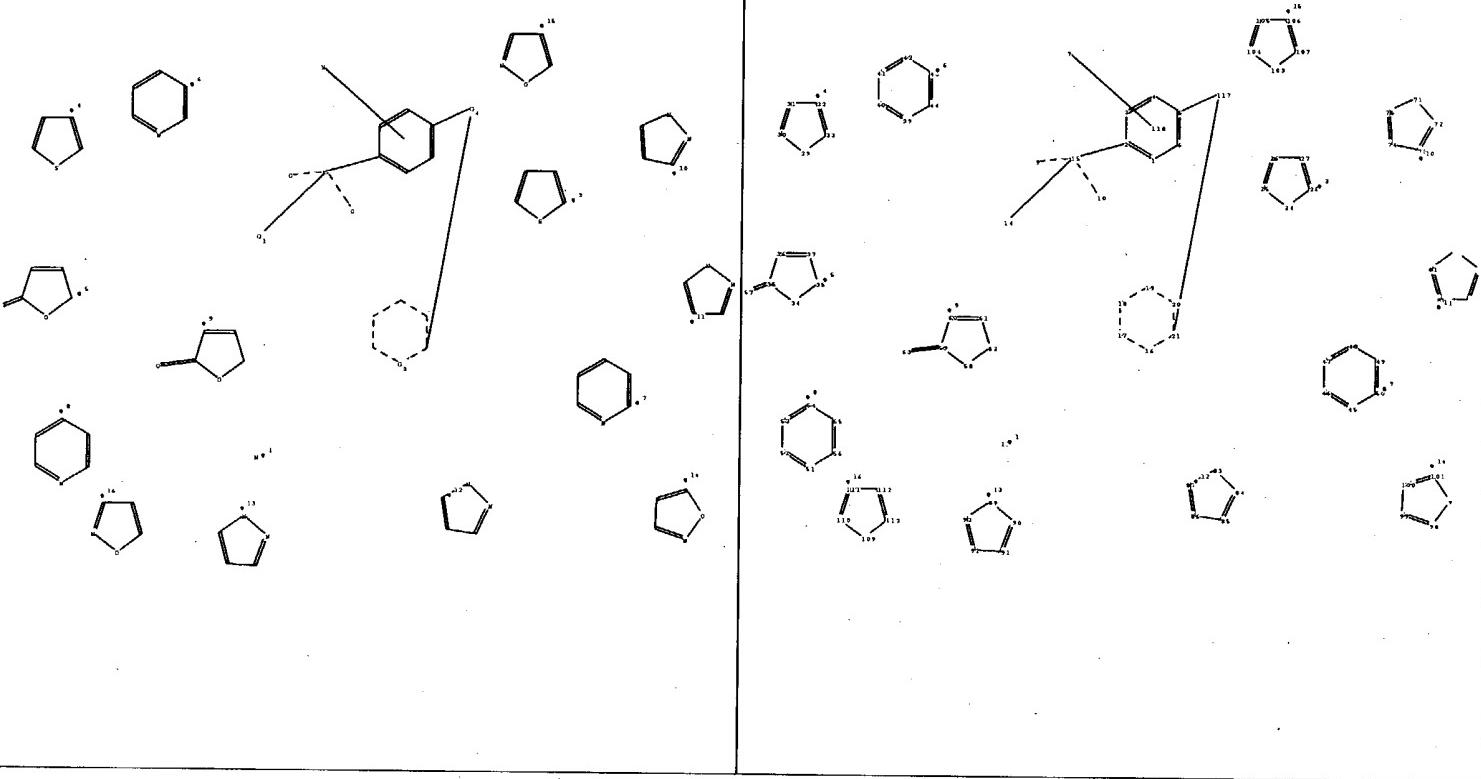
1:CH3,Et,[*1]

G3:C,N

G4:[*1],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15],[*16]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS
12:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom
45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:CLASS
54:CLASS 55:Atom 56:Atom 57:Atom 58:CLASS 59:Atom 60:Atom 61:Atom 62:Atom
63:Atom 64:CLASS 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 78:Atom 79:Atom 80:Atom
81:Atom 82:Atom 84:Atom 85:Atom 86:Atom 87:Atom 88:Atom 90:Atom 91:Atom 92:Atom
93:Atom 94:Atom 98:Atom 99:Atom 100:Atom 101:Atom 102:Atom 104:Atom 105:Atom
106:Atom 107:Atom 108:Atom 110:Atom 111:Atom 112:Atom 113:Atom 114:Atom 118:CLASS



chain nodes :

7 9 10 11 14 15 57 63 117

ring nodes :

1	2	3	4	5	6	16	17	18	19	20	21	24	25	26	27	28	29	30	31	32	33	34	35
36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	58		
59	60	61	62	71	72	73	74	75	77	78	79	80	81	83	84	85	86	87	89	90	91		
92	93	97	98	99	100	101	103	104	105	106	107	109	110	111	112	113							

chain bonds :

2-15 5-117 9-15 10-15 14-15 21-117 35-57 59-63

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	16-17	16-21	17-18	18-19	19-20	20-21	24-25	24-28														
25-26	26-27	27-28	29-30	29-33	30-31	31-32	32-33	34-35	34-38	35-36	36-37	37-38	39-40	39-44	40-41	41-42	42-43	43-44	45-46	45-50	46-47	47-48	48-49	49-50	51-52		
51-56	52-53	53-54	54-55	55-56	58-59	58-62	59-60	60-61	61-62	61-62	71-72	71-75	72-73	73-74	74-75	77-78	77-81	78-79	79-80	80-81	83-84	83-87	84-85	85-86	86-87	89-90	
89-93	90-91	91-92	92-93	97-98	97-101	98-99	99-100	100-101	103-104	103-107	104-105	105-106	106-107	109-110	109-113	110-111	111-112	112-113									

exact/norm bonds :

2-15	5-117	9-15	10-15	14-15	16-17	16-21	17-18	18-19	19-20	20-21	21-117	24-25	24-28	25-26	26-27	27-28	29-30	29-33	30-31	31-32	32-33	34-35	34-38	35-36	35-57	36-37	37-38	58-59	58-62	59-60	59-63	60-61	61-62	71-72	71-75	72-73	73-74	74-75			
77-78	77-81	78-79	79-80	80-81	83-84	83-87	84-85	85-86	86-87	89-90	89-93	90-91	91-92	92-93	97-98	97-101	98-99	99-100	100-101	103-104	103-107	104-105	105-106	106-107	109-110	109-113	110-111	111-112	112-113												

normalized bonds :

1-2	1-6	2-3	3-4	4-5	5-6	39-40	39-44	40-41	41-42	42-43	43-44	45-46	45-50	46-47	47-48	48-49	49-50	51-52	51-56	52-53	53-54	54-55	55-56
-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

isolated ring systems :

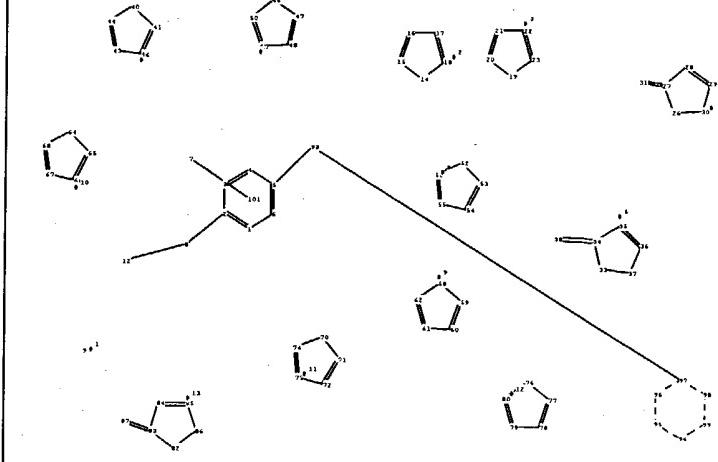
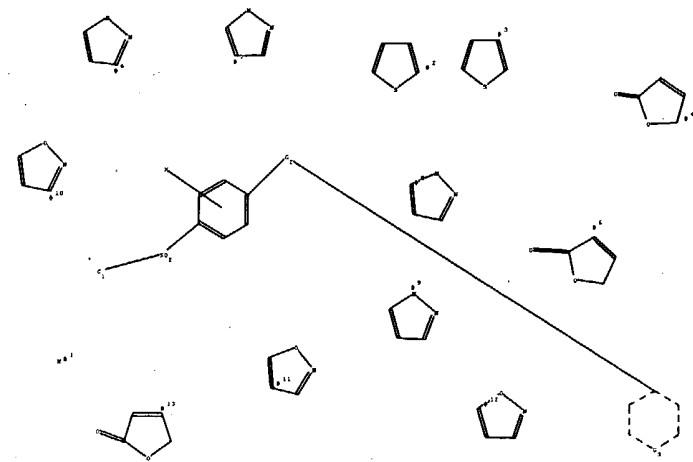
containing 1 : 16 : 24 : 29 : 34 : 39 : 45 : 51 : 58 : 71 : 77 : 83 : 89 : 109 :

G3:C,N

G4:[*1],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13],[*14],[*15],[*16]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS
14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom
45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom
55:Atom 56:Atom 57:CLASS 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS
71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom
83:Atom 84:Atom 85:Atom 86:Atom 87:Atom 89:Atom 90:Atom 91:Atom 92:Atom 93:Atom
97:Atom 98:Atom 99:Atom 100:Atom 101:Atom 103:Atom 104:Atom 105:Atom 106:Atom
107:Atom 109:Atom 110:Atom 111:Atom 112:Atom 113:Atom 117:CLASS 118:CLASS



main nodes :

7 8 9 12 31 38 87 93

ring nodes :

1	2	3	4	5	6	14	15	16	17	18	19	20	21	22	23	26	27	28	29	30	33	34	35
36	37	40	41	42	43	44	46	47	48	49	49	50	52	53	54	55	56	58	59	60	61	62	
64	65	66	67	68	70	71	72	73	74	76	77	78	79	80	82	83	84	85	86	94	95		
96	97	98	99																				

main bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-97

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	14-15	14-18	14-19	15-16	16-17	16-18	17-18	17-19	19-20	19-23	19-24	20-21	20-22	21-22	22-23	
21-22	22-23	26-27	26-30	27-28	27-29	28-29	28-30	29-30	33-34	33-37	33-38	34-35	34-36	35-36	36-37	36-38	36-39	36-40	37-41		
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-54	52-55	53-54	54-55	55-56	56-57	57-58	58-59	59-60	60-61	61-62	
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	68-69	70-71	70-72	71-72	72-73	73-74	74-75	75-76	76-77	77-78	
71-72	72-73	73-74	73-75	76-77	76-80	77-78	77-79	78-79	79-80	82-83	82-84	82-85	83-84	84-85	85-86	86-87	87-88	88-89	89-90	90-91	
94-95	94-96	95-96	96-97	97-98	98-99																

act/norm bonds :

2-8	5-93	8-12	14-15	14-18	14-19	15-16	16-17	16-18	17-18	17-19	19-20	19-23	20-21	21-22	22-23					
26-27	26-30	27-28	27-31	28-29	28-30	33-34	33-37	33-38	34-35	34-36	35-36	36-37	36-38	36-39	36-40					
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-54	52-55	53-54	54-55	55-56	56-57	57-58				
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	68-69	70-71	70-72	71-72	72-73	73-74				
71-72	72-73	73-74	73-75	76-77	76-80	77-78	77-79	78-79	79-80	82-83	82-84	82-85	83-84	83-85	84-85	85-86				
85-86	93-97	94-95	94-96	95-96	96-97	97-98	98-99													

rmalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

olated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

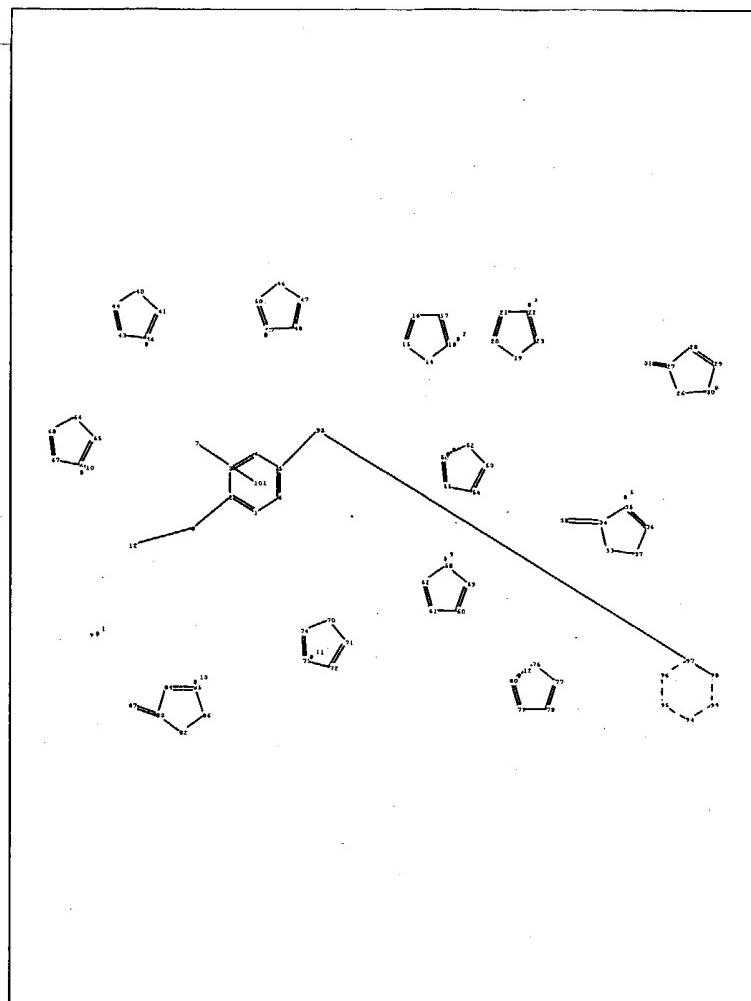
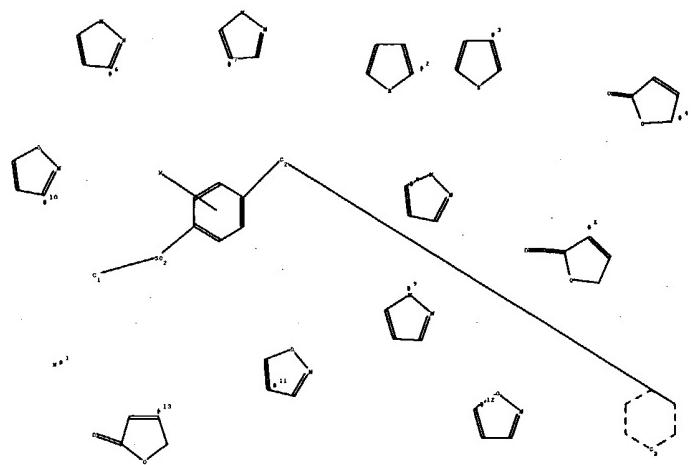
:CH3,Et,[*1]

[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1	2	3	4	5	6	14	15	16	17	18	19	20	21	22	23	26	27	28	29	30	33	34	35
36	37	40	41	42	43	44	46	47	48	49	50	52	53	54	55	56	58	59	60	61	62		
64	65	66	67	68	70	71	72	73	74	76	77	78	79	80	82	83	84	85	86	94	95		
96	97	98	99																				

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-98

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	14-15	14-18	15-16	16-17	17-18	17-19	19-20	19-23	20-21	20-22	21-22	22-23					
21-22	22-23	26-27	26-30	27-28	28-29	29-30	29-30	33-34	33-37	33-37	34-35	35-36	36-37	36-37	36-37	36-37	36-37	40-41				
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-53	52-56	53-54	54-55									
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-71	70-74									
71-72	72-73	73-74	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	84-85	85-86									
94-95	94-99	95-96	96-97	97-98	98-99																	

exact/norm bonds :

2-8	5-93	8-12	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21	21-22	22-23										
26-27	26-30	27-28	27-31	28-29	29-30	33-34	33-37	34-35	34-38	35-36	36-37	36-37	40-41									
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-56	53-54	54-55										
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-74										
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	83-87	84-85	85-86									
85-86	93-98	94-95	94-99	95-96	96-97	97-98	98-99															

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

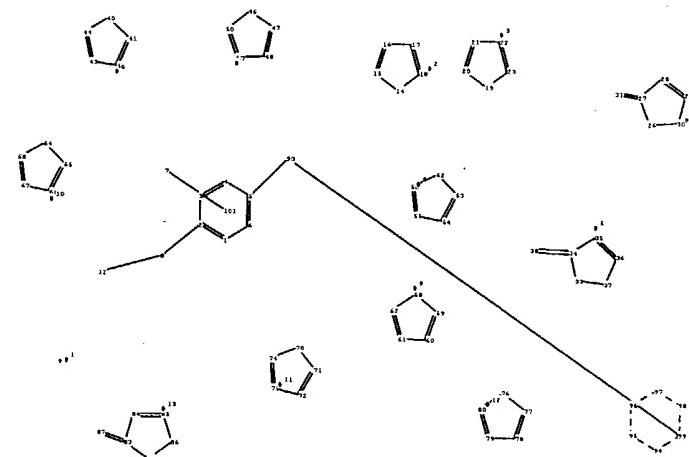
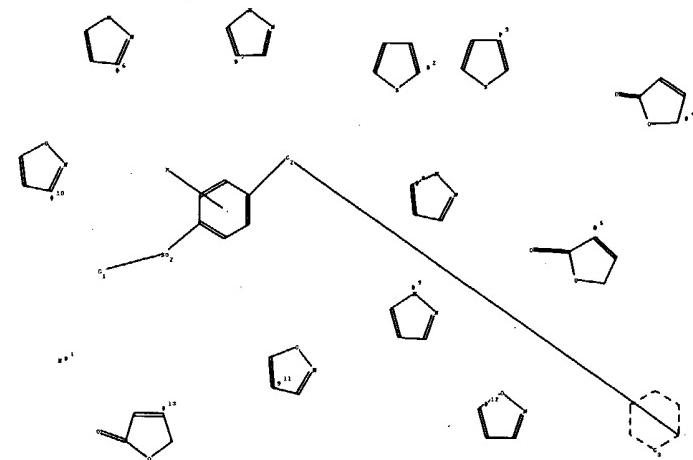
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1	2	3	4	5	6	14	15	16	17	18	19	20	21	22	23	26	27	28	29	30	33	34	35
36	37	40	41	42	43	44	46	47	48	49	49	50	52	53	54	55	56	58	59	60	61	62	
64	65	66	67	68	70	71	72	73	74	76	77	78	79	80	82	83	84	85	86	94	95		
96	97	98	99																				

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-99

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21										
21-22	22-23	26-27	26-30	27-28	28-29	29-30	33-34	33-37	34-35	34-35	35-36	36-37	40-41										
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-53	52-56	53-54	54-55										
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-71	70-74										
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	84-85	85-86											
94-95	94-99	95-96	96-97	97-98	98-99																		

exact/norm bonds :

2-8	5-93	8-12	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21	21-22	22-23											
26-27	26-30	27-28	27-31	28-29	29-30	33-34	33-37	34-35	34-38	35-36	36-37	40-41											
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-53	52-56	53-54	54-55										
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-71	70-74										
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	83-87	84-85	85-86										
85-86	93-99	94-95	94-99	95-96	96-97	97-98	98-99																

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

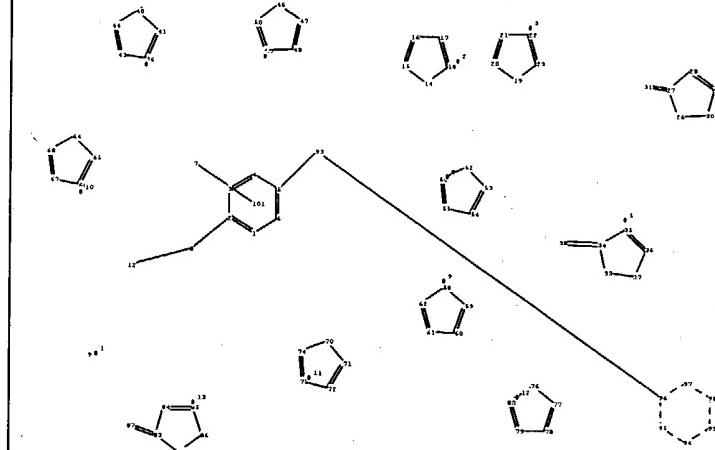
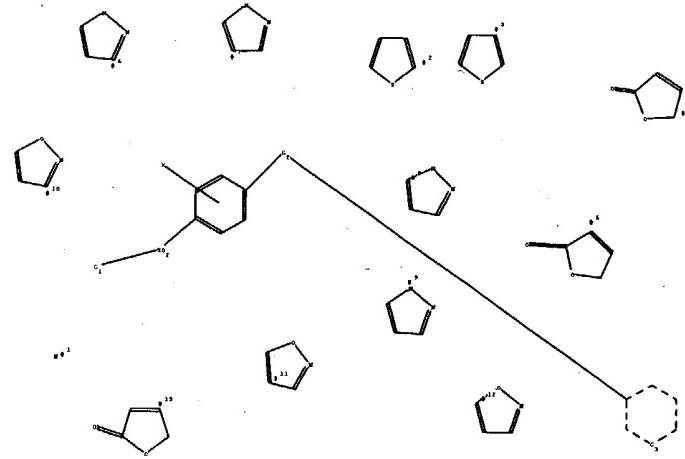
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

atch level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1	2	3	4	5	6	14	15	16	17	18	19	20	21	22	23	26	27	28	29	30	33	34	35
36	37	40	41	42	43	44	46	47	48	49	50	52	53	54	55	56	58	59	60	61	62		
64	65	66	67	68	70	71	72	73	74	76	77	78	79	80	82	83	84	85	86	94	95		
96	97	98	99																				

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-96

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	14-15	14-18	15-16	16-17	16-18	17-18	19-20	19-23	20-21	20-21	21-22	22-23					
21-22	22-23	26-27	26-30	27-28	28-29	29-30	33-34	33-34	33-37	33-37	34-35	35-36	36-37	40-41								
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-53	52-56	53-54	54-55									
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-71	70-74									
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	84-85	85-86										
94-95	94-99	95-96	96-97	97-98	98-99																	

exact/norm bonds :

2-8	5-93	8-12	14-15	14-18	15-16	16-17	16-18	17-18	19-20	19-23	20-21	21-22	22-23									
26-27	26-30	27-28	27-31	28-29	29-30	33-34	33-34	33-37	34-35	34-38	35-36	36-37	40-41									
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-53	52-56	53-54	54-55									
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-71	70-74									
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	83-87	84-85	85-86									
85-86	93-96	94-95	94-99	95-96	96-97	97-98	98-99															

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

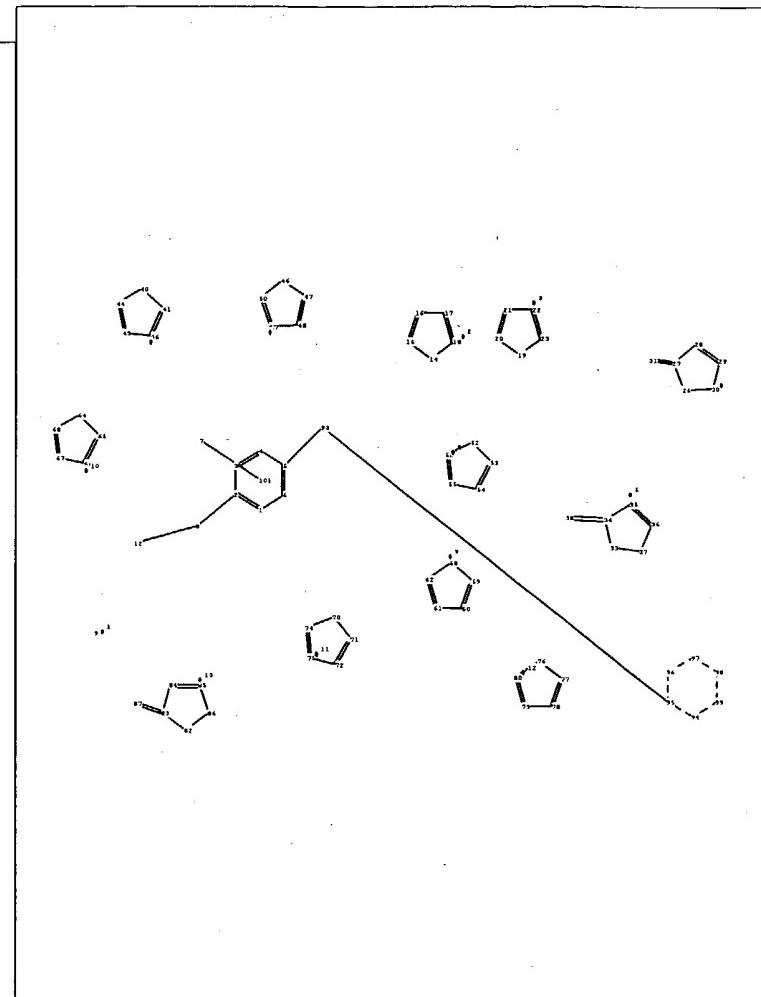
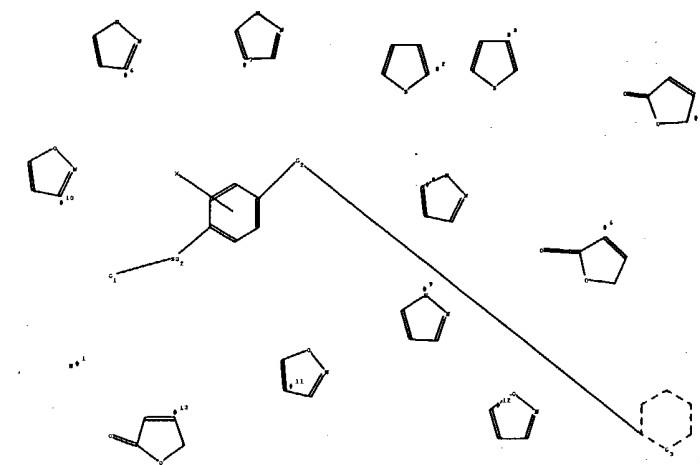
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom
61:Atom 62:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom 71:Atom 72:Atom
73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1	2	3	4	5	6	14	15	16	17	18	19	20	21	22	23	26	27	28	29	30	33	34	35
36	37	40	41	42	43	44	46	47	48	49	49	50	52	53	54	55	56	58	59	60	61	62	
64	65	66	67	68	70	71	72	73	74	76	77	78	79	80	82	83	84	85	86	94	95		
96	97	98	99																				

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87 93-95

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	14-15	14-18	15-16	15-17	16-17	17-18	19-20	19-23	20-21	21-22	22-23	
21-22	22-23	26-27	26-30	27-28	28-29	29-30	33-34	33-37	33-37	34-35	35-36	36-37	40-41				
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-56	53-54	54-55					
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-74					
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	84-85	85-86					
94-95	94-99	95-96	96-97	97-98	98-99												

exact/norm bonds :

2-8	5-93	8-12	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21	21-22	22-23
26-27	26-30	27-28	27-31	28-29	29-30	33-34	33-37	34-35	34-38	35-36	36-37	40-41
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-56	53-54	54-55
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-74
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	83-87	84-85
85-86	93-95	94-95	94-99	95-96	96-97	97-98	98-99					

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

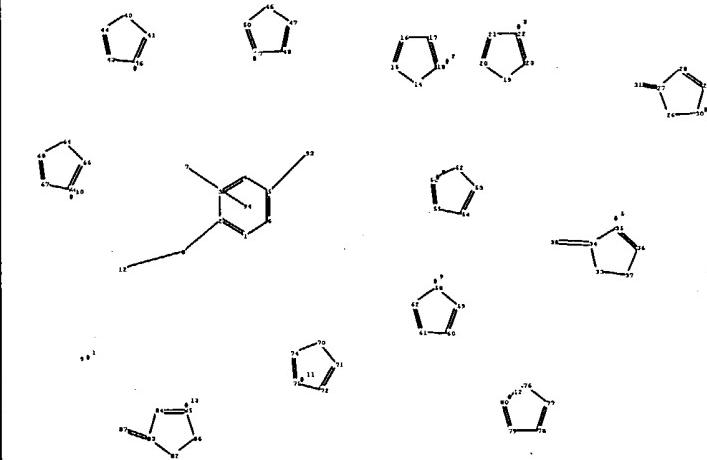
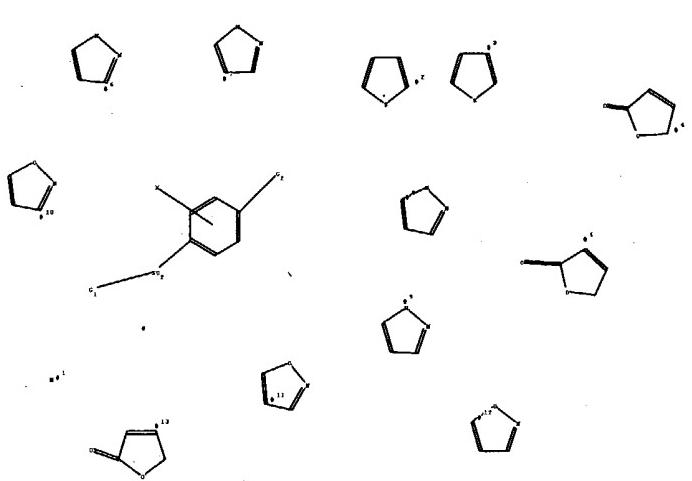
G1:CH3,Et,[*1]

G2:[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]

G3:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
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73:Atom 74:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 82:Atom 83:Atom 84:Atom
85:Atom 86:Atom 87:CLASS 93:CLASS 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom
99:Atom 101:CLASS



chain nodes :

7 8 9 12 31 38 87 93

ring nodes :

1	2	3	4	5	6	14	15	16	17	18	19	20	21	22	23	26	27	28	29	30	33	34	35
36	37	40	41	42	43	44	46	47	48	49	50	52	53	54	55	56	58	59	60	61	62		
64	65	66	67	68	70	71	72	73	74	76	77	78	79	80	82	83	84	85	86				

chain bonds :

2-8 5-93 8-12 27-31 34-38 83-87

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6	14-15	14-18	15-16	16-17	17-18	19-20	19-23	20-21
21-22	22-23	26-27	26-30	27-28	28-29	29-30	33-34	33-37	34-35	35-36	36-37	40-41	
40-44	41-42	42-43	43-44	46-47	46-50	47-48	48-49	49-50	52-53	52-56	53-54	54-55	
55-56	58-59	58-62	59-60	60-61	61-62	64-65	64-68	65-66	66-67	67-68	70-71	70-74	
71-72	72-73	73-74	76-77	76-80	77-78	78-79	79-80	82-83	82-86	83-84	84-85	85-86	

exact/norm bonds :

5-93 8-12 27-31 34-38 40-41 40-44 41-42 46-47 46-50 47-48 52-53 52-56 53-54
58-59 58-62 59-60 65-66 71-72 77-78 83-87

exact bonds :

2-8 14-15 14-18 15-16 16-17 17-18 19-20 19-23 20-21 21-22 22-23 26-27 26-30
 27-28 28-29 29-30 33-34 33-37 34-35 35-36 36-37 42-43 43-44 48-49 49-50 54-55
 55-56 60-61 61-62 64-65 64-68 66-67 67-68 70-71 70-74 72-73 73-74 76-77 76-80
 78-79 79-80 82-83 82-86 83-84 84-85 85-86

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 14 : 19 : 26 : 33 : 40 : 46 : 52 : 58 : 64 : 70 : 76 : 82 :

G1:CH3,Et,[*1]

G2: [*2], [*3], [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 12:CLASS
14:Atom

15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 33:Atom 34:Atom 35:Atom 36:Atom
37:Atom 38:CLASS 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 46:Atom 47:Atom 48:Atom
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85:Atom 86:Atom 87:CLASS 93:CLASS 94:CLASS